Abstract Submitted
for the 4CF11 Meeting of
The American Physical Society

Quasi-Quantum Dynamics of Collinear Reactive Collisions using Operator methods TIM WENDLER, MANUEL BERRONDO, Brigham Young University — We calculate transition probabilities between discrete states of a diatomic molecule induced by an incoming atom. Our prototype Hamiltonian is constructed treating the translation classically and the internal variables quantum mechanically. The corresponding equations of motion are coupled quasi-classically. We present applications to a canonical ensemble of initial conditions as well as results for the time dependence of transition probabilities for different initial and final states. In the reactive case we are driven to using natural coordinates i.e. the reaction coordinate and the transverse vibrational coordinate.

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Date submitted: 14 Sep 2011 Electronic form version 1.4